Cavity (CAV) Package
Users' Guide

The Cavity (CAV) package in MELCOR models the attack on the basemat concrete by hot (often molten) core materials. The effects of heat transfer, concrete ablation, cavity shape change, and gas generation are included. These phenomena may be calculated in more than one location ("cavity") in a MELCOR calculation, and debris may be transferred between cavities. Specific models are described in more detail, with appropriate references, in the Cavity Package Reference Manual. The CAV package has interfaces to the Control Volume Hydrodynamics (CHV) package, the RadioNuclide (RN) package and, through the Transfer Process (TP) package, to the Core (COR) and Fuel Dispersal Interactions (FDI) package.

This Users' Guide gives a brief introduction to the models in the Cavity package, and describes the Cavity package input necessary to run MELGEN and MELCOR. Examples are provided. The available control function arguments, plot variables, and sensitivity coefficients are listed and described. Example input decks for running the Cavity package in MELCOR are provided, as are brief explanations of the printed output and possible error messages.

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1. Model Description

The MELCOR Cavity package is used to model the interactions between core debris and concrete in one or more locations in a MELCOR calculation; modeling is based on the CORCON-Mod3 code. The capabilities of the Cavity package are briefly summarized in this section. More details and references are provided in the Cavity Package Reference Manual.

The physical system considered by the Cavity package consists of an axisymmetric concrete cavity containing debris in one or more layers. The package calculates heat transfer rates from the debris to the concrete and to the top surface of the debris, as well as the heat transfer between layers. After calculating the heat transfer rates, the concrete ablation rate is determined and the ablation products are added to the cavity contents. Chemical reactions involving gaseous products of concrete decomposition (H_2O and CO_2) with the material in the cavity are calculated and the products are transported to the appropriate layer.

Boundary conditions for the top surface of the debris are obtained from an associated control volume in the Control Volume Hydrodynamics (CVH) package, which also serves as a sink for heat and gases released during the interaction. If there is a water pool in the associated volume, it is assumed to overlie the debris; heat transfer to it is calculated using the same full boiling curve employed in CORCON. (The effects of the introduction of gas bubbles at the lower surface of the pool—referred to as "barbotage"—and of subcooling were added in CORCON-Mod3. These enhancements may be disabled, if desired.)

By default, the Cavity package considers all debris, metallic and oxidic, to be mixed into a single layer. However, the user may choose modeling that considers multiple layers. Two options are available. The first, equivalent to modeling in CORCON-Mod2, does not permit mixing of metals and oxides. It allows a maximum of three layers: metal, heavy oxide below the metal, and light oxide above the metal. The second option invokes mechanistic calculations that consider the possibility of mixing heavy oxides into the metals and/or metals into the light oxides by gas flows at their mutual interfaces (in competition with reseparation under gravity).

The user may choose to specify the initial contents of one metal layer and/or one oxide layer, or of a single mixed-phase layer. If both pure layers are specified, their initial orientation will be determined by their calculated densities, with the densest on the bottom and the lightest on top. Subsequent behavior will be determined by the mixing option in effect.

In most cases, however, *no* initial contents will be specified; debris will be deposited into the cavity from the Core (COR) package or the Fuel Dispersal Interactions (FDI) package, through the Transfer Process (TP) package. The user may also specify deposition rates directly by using the External Data File (EDF) package and the TP package. In either case, relative densities and mixing options will determine the layering of the deposited debris.

The decay heat for the cavity can be obtained directly from a user-input control function or calculated using the Decay Heat (DH) and RadioNuclide (RN) packages. In the former case, or if the RN package is not active to track fission-product relocation, two additional user-input control functions must be specified to define the fraction of total decay heat appearing in each phase (oxide and metal). The user may specify these functions in any case, overriding the MELCOR-calculated results. The simple decay heat model from stand-alone CORCON is not available.

If the RN package is active, it will track the radionuclide inventories associated with the debris. Any initial inventory must be specified by input to the RN package on RNFPNijjXX records. When material is transferred into a cavity by the TP package, a parallel transfer of radionuclides is made, also by the TP package. This requires specific input to the TP package, as will be discussed later.

If there is more than one cavity, material may be transferred between cavities. If the RN package is active, the radionuclide inventory associated with the transferred material is also relocated. In this case, the TP package is not involved.

Transfer of material between cavities can be initiated under three types of conditions: axial rupture, radial rupture, or a TRUE value returned from a Control Function. Each of the three types of ruptures (axial, radial, and Control Function) can result in overflow to another cavity, but only “one-way” transfers are allowed between cavities (e.g., cavity 1 can overflow to cavity 2, which then overflows to cavity 3, but cavity 3 cannot overflow back to cavity 1 or 2). Rather than specifying an overflow cavity, if desired, the user can either 1) force the calculation to be stopped when rupture is predicted, or 2) specify that any ruptures will be “ignored” and the calculation continued (with no material transferred out of the cavity) as if additional concrete still remained.

A cavity is considered to have ruptured axially if the basemat is breached and to have ruptured radially if the outer wall is breached. Any material above the elevation at which the rupture occurs will be transferred to a second (user-specified) cavity. The rupture elevation for axial rupture is that of the lowest ablated point, while that for radial rupture is the elevation with minimum remaining wall thickness. Alternatively, the user can control the occurrence of a rupture and the corresponding elevation with Control Functions. If more than one of the three rupture conditions occurs, the one corresponding to the lowest elevation is chosen.

2. User Input

The user input for the Cavity package is described in this section. In MELGEN, one complete set of records is required for each cavity. An arbitrary number of cavities may be defined (subject to total storage available); 100 are permitted by the format of the input records. In MELCOR, certain properties of an *inactive* cavity (one which does not yet contain material) may be altered, but the number of cavities defined in the problem cannot be changed.

2.1 MELGEN Input

A complete set of the following records (at least the required one) must be input for each cavity. They define:

(1) the initial cavity size, shape, concrete type, and contents (if any),

(2) the control volume which provides boundary conditions and the transfer process (if any) which will deposit material into the cavity,

(3) the method for calculating internal (decay) heating, (if not the default), and

(4) miscellaneous control and model parameters,

although not necessarily in that order.

CAVnn00 – Cavity Declaration
$00 \leq nn \leq 99$, nn is the cavity number
Required

This record identifies the control volume associated with each cavity and, if desired, defines a name for the cavity. An optional field allows deactivation of the scrubbing of RN aerosols and/or iodine vapor that are released with cavity gases into overlying CVH water pools.

(1) ICAVN - User number of associated control volume
(type = integer, default = none, units = dimensionless)

(2) CAVNAM - User-defined cavity name
(type = character*16, default = control volume name)

(3) IBUBX - Optional RN pool scrubbing activation flag
(type = integer, default = 0, units = dimensionless)
= 0 RN scrubbing of aerosols and iodine vapor is active

= -1 all RN scrubbing is inactive
= -2 RN scrubbing of aerosols only is active
= -3 RN scrubbing of iodine vapor only is active

CAVnnm0 – Initial Layer Definition
$00 \leq nn \leq 99$, nn is the cavity number
$1 \leq m \leq 9$, m is the layer number, used for input only
Optional

This record can be used to specify that material will be present in cavity nn at the start of a calculation. Normally, material is not present in the cavity at the start of a calculation, but is introduced into the cavity during the transient from the other packages of MELCOR.

If it is desired to begin a calculation with material in cavity nn, the initial temperature for each layer in the cavity must be entered on a CAVnnm0 record. One layer containing only metals and/or one layer containing only oxides, *or* a single layer containing both metals and oxides may be defined. No use is made of the actual value or values input for m; the ordering of the layers, if there are two, will be determined by their calculated densities.

If elimination of a layer that was defined in a previous version of the input deck is desired, this record can also be used to delete it. (Note that if the replacement feature of the input processor is used, only the *last* CAVnnm0 record in the input stream will be used.) Any CAVnnmx records with the same m will then be ignored.

<u>Form 1, defining a layer:</u>

(1) - Keyword. The character variable TEMP must be entered.
(type = character, default = none)

(2) TEMP - Initial temperature of layer
(type = character, default = none, units = K)

<u>Form 2, deleting a layer:</u>

(1) - Keyword. The character variable DELETE must be entered.
(type = character, default = none)

CAVnnmk – Layer Contents
$00 \leq nn \leq 99$, nn is the cavity number, m is the layer number
$1 \leq m \leq 9$, m is the layer number, used for input only.
$1 \leq k \leq 9$
Required, if record CAVnnm0 (first form) is present

These records specify the initial layer contents. There can be up to 9 of them, with each record consisting of one or more pairs of data. The first entry of each pair is a character variable identifying a species and the second entry is a real variable that specifies the initial mass of the species. Multiple data pairs can be specified on a record, but pairs cannot be split between records. No more than two layers are permitted, as discussed above.

For each data pair:

(1) - Keyword identifying species. Possible values include AL2O3, CAO, CR2O3, FEO, NIO, SIO2, UO2, ZRO2, AL, C(C), CR, FE, NI, U, and ZR. Other species listed in Appendix A of the Cavity Package Reference Manual may also be used.
(type = character, default = none)

(2) SPMASS - Initial mass of material
(type = real, default = none, units = kg)

CAVnnC0 – Concrete Declaration

00 ≤ nn ≤ 99, nn is the cavity number
Required

This record specifies the type of concrete in the cavity. There are three options:

Form 1, Standard concrete from CORCON:

(1) - Keyword. The character variable CORCON must be entered.
(type = character, default = none)

(2) ICON - CORCON concrete type (type = character, default = none)
= 1 Basaltic aggregate concrete
= 2 Limestone aggregate/common sand concrete
= 3 Generic SE United States concrete
= 4 Savannah River Site concrete

Form 2, Standard concrete with simplified composition:

(1) CONTYP - Type of concrete in cavity
(type = character*16, default = none)
= BASALT basaltic concrete
= LIMESTONE/CS limestone/common sand concrete
= CRBR Clinch River Breeder Reactor concrete

Form 3, Nonstandard concrete:

(1) CONTYP - Name of nonstandard concrete type
(type = chraacter*16, default = USER-INPUT)

CAVnnCk – Concrete Composition

00 ≤ nn ≤ 99, nn is the cavity number
1 ≤ k ≤ 9
Required if CONTYP is not a standard composition
Otherwise, optional to modify standard composition

There can be up to 9 of these records. The data are entered in pairs consisting of a character keyword and a real number. The keyword identifies the species and the real number specifies the species mass fraction in the concrete. Multiple data pairs can be specified on a record, but pairs cannot be split between records.

Reinforcing bars are considered part of the concrete composition in MELCOR, unlike stand-alone CORCON. The default compositions for standard concretes contain no rebar; therefore, the rebar content should be included as part of these data, even for standard concretes. The composition is not limited to iron. This feature can be used to model metal inserts in the concrete in some experiments.

If a nonstandard composition was specified for CONTYP, these records specify the concrete composition. For this case, unnormalized mass fractions may be entered.

If a standard concrete type was specified for CONTYP, its default composition is given in Table 2.1. The CAVnnCk record can be used to modify the default composition (e.g., to add rebar or to modify the water content). For this case, the specified (input) mass fraction(s) for the material(s) being modified will be used directly, and the mass fraction(s) of all other materials contained in the standard composition will be renormalized so that the sum of the mass fractions of all of the concrete materials will equal 1.

For each data pair:

(1) - Keyword identifying species. Possible values include AL2O3, CAO, CR2O3, FEO, NIO, SIO2, UO2, ZRO2, AL, C(C), CR, FE, NI, U, and ZR. Other species listed in Appendix A of the Cavity Package Reference Manual may also be used.
(type = character, default = none)

(2) XMFRCT - Mass fraction of material.
(type = real, default = none, units = dimensionless)

Table 2.1 Default Concrete Compositions (in mass %)

SPECIES	CORCON				BASALT	LIMESTONE/CS	CRBR
	1	2	3	4			
SIO2	54.84	35.80	3.60	67.05	65.00	36.00	4.00
TIO2	1.05	0.18	0.12	1.00	.	.	.
MNO	.	0.03	0.01	.	.	.	.
MGO	6.16	0.48	5.67	2.68	.	.	.
CAO	8.82	31.30	45.40	13.41	.	.	.
NA2O	1.80	0.082	0.078	1.00	.	.	.
K2O	5.39	1.22	0.68	1.00	.	.	.
FE2O3	6.26	1.44	1.20	1.00	.	.	.
AL2O3	8.32	3.60	1.60	6.26	20.00	5.00	3.00
CR2O3	.	0.014	0.004	.	.	.	.
CO2	1.50	21.154	35.698	1.50	.	.	.
H2OCHEM	2.00	2.00	2.00	2.00	.	.	.
CACO3	.	.	.	.	3.00	48.00	81.00
CA(OH)2	.	.	.	.	8.00	8.00	8.00
H2OEVAP	3.86	2.70	3.94	3.10	4.00	3.00	4.00

CAVnnCa – Other Concrete Properties

$00 \leq nn \leq 99$, nn is the cavity number

$A \leq a \leq Z$

All except TINCT and EMISCT are required if CONTYP is not a standard composition. Defaults for standard concretes are given in Table 2.2.

There can be up to 26 of these records, with data entered in pairs consisting of a character keyword and a real number. The keyword identifies a concrete property and the real number specifies the value of the property. Multiple data pairs can be specified on a record, but pairs cannot be split between records. Default values are available for the standard concrete types (values are listed below), but these defaults should not be considered as recommended values. The character keywords and corresponding variables are:

DENSCT - Density of concrete.
(type = real, units = kg/m^3, default = Table 2.2 for standard concrete, none for other concrete)

TSOLCT - Solidus temperature of concrete.
(type = real, units = K, default = Table 2.2 for standard concrete, none for other concrete)

TLIQCT - Liquidus temperature of concrete.
(type = real, units = K, default = Table 2.2 for standard concrete, none for other concrete)

TABLCT - Ablation temperature of concrete.
(type = real, units = K, default = Table 2.2 for standard concrete, none for other concrete)

TINCT - Initial temperature of concrete.
(type = real, default = 298.0, units = K)

EMISCT - Emissivity of concrete.
(type = real, default = 0.6, units = dimensionless)

Table 2.2 Default Concrete Properties

PROPERTY	CORCON				BASALT	LIMESTONE/CS	CRBR
	1	2	3	4			
DENSCT (kg/m^3)	2340.	2340.	2340.	2400.	2400.	2340.	2340.
TSOLCT (K)	1350.	1420.	1690.	1353.	1350.	1420.	1690.
TLIQCT (K)	1650.	1670.	1875.	1653.	1650.	1670.	1875.
TABLCT (K)	1450.	1500.	1750.	1450.	1450.	1500.	1750.

CAVnnDH – Control Functions for Decay Heat
$00 \leq nn \leq 99$, nn is the cavity number
Optional

By default, the decay heat power input to the cavity is determined by MELCOR using the inventory of radionuclides in the cavity (calculated by the RN package) and their specific decay powers (defined by the DCH package). If the RN package is inactive (as in analysis of a simulation experiment) or if the user wishes to override or modify its results, control functions may be specified on this record which will then be used in calculation of the decay heat. This provides the capability to define a total decay heat other than that calculated by MELCOR and/or to define the partition of heat input among layers in the pool.

Unless IPDHCF = -1 and the RN package is active, both IPOXCF and IPMCF must be specified ≥ 0 as MELCOR has no other way to determine the partition of heating between layers.

(1) IPDHCF - Flag for total decay heat.
(type = integer, default = none)

< -1 Set decay heat to zero.

= -1 Use calculation from decay heat and radionuclide packages.

≥ 0 Number of the control function which defines the total decay heat in the cavity.

(2) IPOXCF - Flag for fraction of heat in oxide phase.
(type = integer, default = none)

< 0 Use split calculated by MELCOR

≥ 0 Number of control function which specifies fraction of total decay heat to be put into the oxide phase

(3) IPMCF - Flag for fraction of heat in metal phase.
(type = integer, default = none)

< 0 Use split calculated by MELCOR

≥ 0 Number of control function which specifies fraction of total decay heat to be put into the metal phase

CAVnnDL – Ablation Delay
$00 \leq nn \leq 99$, nn is the cavity number
Optional

This record may be used to delay the start of concrete ablation until a user-defined criterion is met in addition to the requirements of the CORCON model. It may be used to model such phenomena as the burn-through of a steel liner. If this record is present, the possibility of ablation will not be considered until the specified logical control function becomes .TRUE.

If the control function is already .TRUE. in MELGEN, a warning will be issued. If, during MELCOR time advancement, the function is .TRUE. and there is material in the cavity, ablation will be considered for that timestep and all subsequent ones. A “latch” is set within the Cavity package so that further changes in the control function will be ignored.

(1) IPDEL - Number of a logical control function to define an additional criterion that must be met before ablation will be calculated.
(type = integer, default = none)

CAVnnG0 – Cavity Geometry
00 ≤ nn ≤ 99, nn is the cavity number
Required

This record specifies the initial geometry of the concrete cavity. The only option available at this time is the “flat-bottom cylinder” option of CORCON. Note that CORCON uses its own coordinate system, with z positive **down**, which is currently totally independent of the rest of MELCOR.

(1) CORCON - Keyword. The character variable CORCON must be entered.
(type = character, default = none, units = dimensionless)

(2) IGEOM - CORCON geometry type. The value 2 must be entered.
(type = integer, default = none)

CAVnnG1 – Parameters of CORCON Coordinate System
00 ≤ nn ≤ 99, nn is the cavity number
Required

(1) NRAYS - Number of rays in CORCON system (≤ 100)
(type = integer, default = none, units = dimensionless)

(2) RO - Radial coordinate of center of ray system. The value 0. must be entered.
(type = real, default = none, units = m)

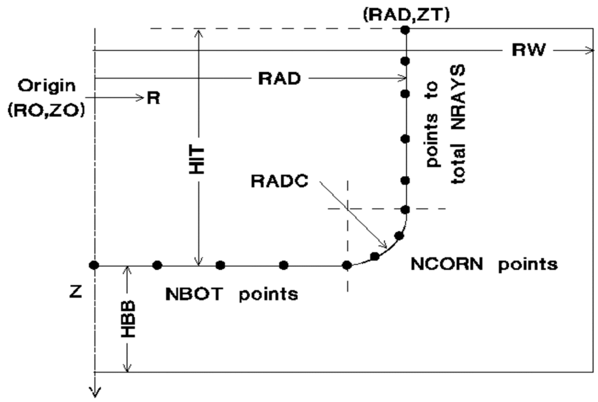
(3) ZO - Axial coordinate of center of ray system
(type = real, default = none, units = m)

CAVnnG2 – Cavity Shape

00 ≤ nn ≤ 99, nn is the cavity number

Required

This record specifies the initial cavity shape. The associated variables are illustrated in the figure below, where NBOT=5, NCORN=2, and NRAYS=13.



(1) ZT - Z coordinate of cylinder top edge
(type = real, default = none, units = m)

(2) RAD - Radius of cylindrical activity
(type = real, default = none, units = m)

(3) HIT - Height of cylindrical cavity
(type = real, default = none, units = m)

(4) RADC - Radius of corner (transition from cylindrical wall to floor) of cavity
(type = real, default = none, units = m)

(5) RW -
- > 0 External radius of concrete
(type = real, default = none, units = m)
- ≤ 0 Negative of number of Tabular Function that defines external radius of concrete as a function of z
(type = real, default = none, units = dimensionless)

(6) HBB - Thickness of concrete below bottom of cavity
(type = real, default = none, units = m)

(7) NBOT - Number of points defining flat bottom of cavity, ≥ 2
(type = integer, default = none, units = dimensionless)

(8) NCORN - Number of points defining corner
(type = real, default = none, units = dimensionless)

CAVnnGa – Additional Geometry Points
A $\leq$ a $\leq$ Z, used for sequencing
Optional

There may be up to 26 of these records, with data entered in triplets. Each triplet is used to add one or more points to the geometry description above the top of the cavity, as previously specified, with decreasing z coordinates in the upward direction. The total number of points may not exceed the maximum of 100. More than one triplet can be specified on a record, but triplets cannot be split between records. If multiple triplets are specified, each must define points lying above all previous points (with records ordered according to the final character, a, of the identifier). In each triplet, the variables are

NEXTRA - Number of points to be added. If NEXTRA > 1, the points will be uniformly spaced along a line segment from the old last point to the new one.
(type = integer, default = none, units = none)

REXTRA - R coordinate of new last point
(type = real, default = none, units = m)

ZEXTRA - Z coordinate of new last point
(type = real, default = none, units = m)

CAVnnRa – Rupture/Overflow Input
00 $\leq$ nn $\leq$ 99, nn is the cavity number
a = R, A, or T
Optional

This record identifies the cavity to which material will be moved if the present cavity ruptures, and optionally identifies Control Functions to control when rupture will occur and the elevation of the rupture. Any combination of the three different types of rupture may be specified: axial (a = A), radial (a = R), or Control Function (a = T). The tests for each type of rupture are discussed in Section 1.

(1) NOVC - User number of the cavity that will receive overflowing material following a rupture. Setting NOVC to -1 signals MELCOR to stop the calculation if this type of rupture occurs. Setting NOVC to -2 specifies that the calculation should continue unchanged (as if infinite concrete were available), even if rupture is predicted
(type = integer, default = -1, units = dimensionless)

(2) NCFRUP - Number of the logical Control Function that will trigger rupture of this cavity. This input is optional for a = A or R, and required for a = T (see Section 1 for further details)
(type = integer, default = none, units = dimensionless)

(3) NCFREL - Number of the real-valued Control Function that specifies the rupture elevation for this cavity. Note that the elevation must be given in the CORCON coordinate system (positive downward). This input is optional for a = A or R, and required for a = T (see Section 1 for further details)
(type = integer, default = none, units = dimensionless)

CAVnnSP – Definition of Parametric Debris Spreading
$00 \leq nn \leq 99$, nn is the cavity number
Optional

This record may be used to model spreading of debris in the cavity. It requires that the user define a maximum debris radius as a function of time through a Tabular Function, Control Function, or channel of an external data file.

The second field on the record is optional. If it is absent, heat transfer from the radial surface of the spreading debris will be considered. If it is present, the only permitted value is ADIABATIC, which will result in suppression of the heat transfer calculation for this surface.

(1) SOURCE - Source of data for maximum debris radius as a function of time.
(type = character, default = none, units = dimensionless)
= TF.nnn Data from tabular function nnn.
= CF.nnn Data from control function nnn.
= EDF.nnn.m Data from channel m of external data file nnn.

(2) HTSIDE - Treatment of heat transfer from radial face of spreading debris.
(type = character, default = heat transfer activated, units = dimensionless)
= ADIABATIC Heat transfer suppressed.

CAVnnTP – Out Transfer Process Number
$00 \leq nn \leq 99$, nn is the cavity number
Optional

This record identifies the “out” transfer process number for transferring mass from the COR or FDI packages to the cavity. If absent, no mass will be transferred into the cavity from the core or fuel debris interactions packages.

(1) NTPOT - "Out" transfer process number ("nnn" on the TPOTnnn00 record) associated with the "in" transfer process for masses and energies from the COR or FDI package.
(type = integer, default = none, units = dimensionless)

Note that this requires input to the TP package. The appropriate input on the TPOTnnn00 record is NMSOT = 5, NPOTOI = "in" process number on either the COR00004 record or the FDInn00 record as appropriate. For transfer from FDI, a unity translation matrix should be used (OUTMTX=DEF.1). For transfer direct from COR, a user-defined matrix should be used (OUTMTX = UIN.mmm, where "mmm" is the number of the translation matrix), the corresponding TPMmmm0000 record should define NROW = 5 and NCOL = 6 (the Cavity package does nothing with control poison from the core), and the remaining TPMmmm… records should define matrix elements 1/1, 2/2, 3/3, 4/4, and 5/5 equal to 1.0.

In order to transfer the radionuclides along with the total masses, additional Transfer Process numbers must be defined. Currently, these radionuclide TP numbers must be exactly 500 greater than the corresponding TP numbers defined for total mass and energy transfers by the COR or FDI and CAV input. The appropriate TP parameters are a number of masses (which is equal to the total number of radionuclide classes), NTHERM = 1, and a unity translation matrix (DEF.1 on the TPOTnnn00 record).

CAVnnak – Miscellaneous Control and Model Parameters
$0 \leq nn \leq 99$, nn is the cavity number
$U \leq a \leq Z$
k arbitrary
Optional

There can be up to 216 of these records with data entered in pairs consisting of a character keyword and either a real or integer variable. The keyword identifies the parameter and the real or integer variable specifies the value of the parameter. Multiple data pairs can be entered on a record, but data pairs cannot be split between records.

The character variables are:

BOILING - Treatment of enhancements to the boiling curve for heat transfer to overlying coolant. A multiplier may be applied to the standard curve (including subcooling and gas barbotage enhancements), or the enhancements may be suppressed.
(type = real, default = 0., units = none)
= 0. Use standard CORCON-Mod3 model, including enhancements

> 0. Use value as multiplier on standard model
< 0. Suppress enhancements (the CORCON-Mod2 model)

COKE - Coking flag. A value of zero will enable production of condensed carbon during oxidation of zirconium. If enabled by previous input, a non-zero value will suppress the reaction.
(type = real, default = 1., units = none)

CTOXYREA - Treatment of chemical reactions involving concrete decomposition products. Any non-zero value will suppress the reduction of ablated oxides by debris metals. If suppressed by previous input, a value of zero will enable the reaction.
(type = real, default = 0., units = none)
= 0. Include oxides and gases as reactants
≠ 0. Exclude oxides, and consider gases only (the CORCON-Mod2 model)

EMISS.OX - Emissivity of the oxide phase.
(type = real, default = 0.6, units = dimensionless)

EMISS.MET - Emissivity of the metal phase.
(type = real, default = 0.6, units = dimensionless)

EMISS.SUR - Emissivity of the surroundings.
(type = real, default = 0.6, units = dimensionless)

GFILMBOTT - Selection of gas or slag film model for the melt/concrete interface at the bottom surface of the debris. Any non-zero value selects the gas film model.
(type = real, default = 1., units = none)
= 0. Use slag film model
≠ 0. Use gas film model (the CORCON-Mod2 model)

GFILMSIDE - Selection of gas or slag film model for the melt/concrete interface at the radial surface of the debris. Any non-zero value selects the gas film model.
(type = real, default = 1., units = none)
= 0. Use slag film model
≠ 0. Use gas film model (the CORCON-Mod2 model)

HTRBOT - Treatment of debris-to-surface heat transfer at the bottom surface of the debris. Either a multiplier on the standard model or an alternate analytic form may be specified.
(type = real, default = 0., units = dimensionless)

= 0. Use standard CORCON-Mod3 model
> 0. Use value as multiplier on standard model
< 0. Use alternate form of correlation with coefficients defined by sensitivity coefficients C2309(1-3)

HTRINT - Treatment of debris-to-surface heat transfer at interior interfaces between debris layers. Either a multiplier on the standard model or an alternate analytic form may be specified.
(type = real, default = 0., units = dimensionless)
= 0. Use standard CORCON-Mod3 model
> 0. Use value as multiplier on the standard model
< 0. Use alternate form of correlation with coefficients defined by sensitivity coefficients C2309(7-9)

HTRSIDE - Treatment of debris-to-surface heat transfer at the radial surface of the debris. Either a multiplier on the standard model or an alternate analytic form may be specified.
(type = real, default = 0., units = dimensionless)
= 0. Use standard CORCON-Mod3 model
> 0. Use value as multiplier on the standard model
< 0. Use alternate form of correlation with coefficients defined by sensitivity coefficients C2309(4-6)

MIXING - Treatment of mixing between metallic and oxidic components of the debris.
(type = real, default = -1., units = none)
= 0. Suppress mixing (the CORCON-Mod2 model)
> 0. Calculate mixing and separation rates from correlations
< 0. Enforce mixing (all debris forms a single mixed layer)

NONIDEAL - Treatment of chemical free energies in the VANESA fission product release model. Because the nonideal oxide model is not operational, options invoking it cannot be used.
(type = real, default = -1., units = none)
= 0. Nonideal model for both metals and oxides - not available for use
> 0. Ideal model for both metals and oxides
= -1. Nonideal model for metals, ideal model for oxides
= -2. Ideal model for metals, nonideal model for oxides - not available for use

RADLEN - Path length for the optional aerosol opacity calculation in the calculation of radiative heat loss from the debris surface.
(type = real, default = 0., units = m)

SHAPEPLOT - Inclusion of cavity shape data in the plot file in the form of r and z coordinates of the defining body points. By default these are omitted to reduce the size of the plot file. (see Section 4 for details)
(type = real, default = 0., units = none)
= 0. Exclude cavity shape data from plot file
$\neq$ 0. Include cavity shape data in plot file

TDEBUG - Time to start CORCON diagnostic print.
(type = real, default = “infinity”, units = s)

2.2 MELCOR Input

Certain elements of the input for an application of the cavity model may be modified at a restart *if the model is not yet active (if the cavity contains no material)*. These allow changes to initial geometry, concrete type, and miscellaneous model parameters. This is intended to allow a user to perform several calculations which vary on cavity parameters without the need to rerun the pre-vessel-failure part of the calculation.

In addition, cavity rupture/overflow input can be changed such that a cavity continues to ablate (without any material being transferred out of it) even if rupture is predicted. This change can be made even if a cavity is already active.

The input is a subset of that described for MELGEN; the permitted records are listed below (any others will be ignored). Details for each record are provided in Section 2.1.

CAVnn00 – Cavity Declaration
Only the cavity name may be changed from MELGEN.

CAVnnC0 – Concrete Declaration

CAVnnCk – Concrete Composition

CAVnnCa – Other Concrete Properties
If CAVnnC0 is present, a complete concrete definition must be included. If CAVnnC0 is absent, other CAVnnC* records will be ignored.

CAVnnG0 – Cavity Geometry

CAVnnG1 – Parameters of CORCON Coordinate System

CAVnnG2 – Cavity Shape

If CAVnnG0 is present, all of the following records must be included, even though the data elements involved may be unchanged from MELGEN, If CAVnnG0 is absent, other CAVnnG* records will be ignored.

CAVnnGa – Additional Geometry Points

This may not be included without CAVnnG0, CAVnnG1, and CAVnnG2, even if these involve no changes from MELGEN.

CAVnnRa – Rupture/Overflow Input

The only overriding change permitted is to change NOVC to -2. NCFRUP and NCFREL need not be entered. If they are, they must be identical to the values previously input to MELGEN.

CAVnnak – Miscellaneous Model and Control Parameters

Any appropriate combination described in the preceding section may be entered, whether or not present in MELGEN input.

3. Sensitivity Coefficients

The sensitivity coefficients for the Cavity package have identifier numbers from 2300 to 2499. Sensitivity coefficient array 2301, recognized by MELCOR 1.8.2, was eliminated in favor of similar capabilities available through a new array, 2309, in MELCOR 1.8.3. Most of the other sensitivity coefficients from previous versions of the CAV package (specifically, 2302, 2304, 2305, part of 2306, 2307, and 2308), have not yet been connected to CORCON-Mod3. This situation will be corrected in later versions of MELCOR.

2300 – Ablation Enthalpy

This coefficient may be used to modify the heat of ablation of concrete. At this time, it has no effect on restart unless the concrete is also redefined.

The heat of ablation is defined herein as the heat required to convert a unit mass of virgin concrete <u>at the user-specified initial temperature</u>, to condensed-phase and gaseous decomposition products, all at the specified ablation temperature. It contains contributions <u>from sensible heat</u>, heat of chemical decomposition, and heat of fusion, and is internally calculated from the CORCON thermochemical database. It is important to realize that all enthalpies are calculated from the *same* database. Therefore, while increasing the ablation temperature will increase the value calculated for the heat of ablation, it will lead to an equal reduction in the heat necessary to raise the ablation products to a given pool temperature. Thus, the net effect of a change in ablation temperature on the heat necessary to ablate a unit mass of concrete and bring the ablation products to pool temperature is only indirect, through a possible change in the pool temperature predicted. In order to change the energy balance associated with ablation, it is necessary to modify the heat of ablation *at a given ablation temperature*.

(1) - Additional ablation enthalpy to be added to internally-calculated value. (default = 0.0, units = J/kg, equiv = DDELH)

2306 – Heat Transfer, Above Melt

These coefficients may be used to modify heat transfer from the surface of the debris pool.

(1) - Convective heat transfer coefficient in atmosphere. (default = 10.0, units = W/m^2K, equiv = HA)

(2) - Convective heat transfer coefficient in water pool. (default = 1000.0, units = W/m^2K, equiv = HCONV)

2309 – Heat Transfer, Layer Bulk to Interface

These coefficients may be used to modify the coefficients in the alternate correlations used for gas-enhanced heat transfer between the interior of a liquid layer (or sublayer) and its surfaces. These alternate correlations are selected by the HTRBOT, HTRINT, and HTRSIDE keywords on CAVnnak records. (Note that the model also includes natural convection and conduction limits which are *not* modifiable through these coefficients.)

The alternate correlation has the form

$$Nu = A * Re^B * Pr^C$$

Here the length scale in the Nusselt and Reynolds numbers is the bubble radius. The velocity in the Reynolds number is the superficial velocity of gas flowing through the layer. The alternate correlation has the form used for bottom and interfacial heat transfer in CORCON-Mod2, and the default values for the coefficients are those used there. Differences in evaluation of materials properties in CORCON-Mod3, however, will result in differences in calculated heat transfer. Also, CORCON-Mod2 used a different correlation for side heat transfer. Although detailed agreement is impossible, the default coefficients A, B, and C have been chosen to give heat transfer coefficients in rough agreement with those in CORCON-Mod2 for a limited number of cases.

(1) - Constant A for bubble injection (at the bottom of lowest layer).
(default = 5.05, units = dimensionless, equiv = CCAHTB)

(2) - Exponent B for bubble injection.
(default = 0.5, units = dimensionless, equiv = CCBHTB)

(3) - Exponent C for bubble injection.
(default = 0.8, units = dimensionless, equiv = CCCHTB)

(4) - Constant A for side heat transfer.
(default = 2.0, units = dimensionless, equiv = CCAHTS)

(5) - Exponent B for side heat transfer.
(default = 0.3, units = dimensionless, equiv = CCBHTS)

(6) - Exponent C for side heat transfer.
(default = 0.0, units = dimensionless, equiv = CCCHTS)

(7) - Constant A for interfaces between layers.
(default = 5.05, units = dimensionless, equiv = CCAI)

(8) - Exponent B for interfaces between layers.
(default = 0.5, units = dimensionless, equiv = CCBI)

(9) - Exponent C for interfaces between layers.
(default = 0.8, units = dimensionless, equiv = CCCI)

4. Plot Variables and Control Function Arguments

The Cavity package variables that may be used for plot variables and control function arguments are listed and described below. The control function arguments are denoted by a ‘c’. The plot variable arguments are denoted by a ‘p’. The ‘c’ or ‘p’ characters are inside slashes ‘/’ following the variable name. In the following list, n refers to the cavity number ($0 \leq n \leq 99$), “lay” refers to the desired layer, with HOX referring to the heavy oxide layer, LOX to the light oxide layer, MET to the metal layer, HMX to the heavy mixture layer, and LMX to the light mixture layer. Here “heavy” and “light” are in comparison to the metal. Finally “gas” refers to one of the four gases (H2, H2O, CO, or CO2), and “spc” to one of the condensed-phase species (oxides and metals) in the CORCON species list.

CAV-ACTIVe.n	/c/	Activity flag for cavity n. (logical)
CAV-MTOT.n	/p/	Total mass in cavity n. (units = kg)
CAV-HTOT.n	/p/	Total enthalpy for cavity n. (units = J)
CAV-DHR.n	/cp/	Decay heat rate for cavity n. (units = W)
CAV-MASS.spc.n	/c/	Total mass of requested condensed-phase species in cavity n (summed over all debris layers). (units = kg)
CAV-M.lay.n	/p/	Mass of layer. (units = kg)
CAV-T.lay.n	/cp/	Layer temperature. (units = K)
CAV-RHO.lay.n	/p/	Layer density. (units = kg/m^3)
CAV-THICK.lay.n	/cp/	Layer thickness. (units = m)
CAV-VOL.lay.n	/cp/	Volume occupied by layer. (units = m^3)
CAV-VF.lay.n	/p/	Layer void fraction. (units = dimensionless)
CAV-MAXRAD.n	/cp/	Maximum cavity radius. (units = m)
CAV-MINALT.n	/cp/	Minimum cavity altitude. (units = m)
CAV-TMEX.n	/p/	Total mass of gas released from cavity n. (units = kg)
CAV-MEX.gas.n	/cp/	Total mass of requested gas released from cavity n. (units = kg)
CAV-QREA.n	/cp/	Heating rate by chemical reactions in cavity n. (units = W)
CAV-QCNCT.n	/cp/	Heat loss to concrete in cavity n. Under the assumptions of CORCON-Mod2, this heat goes to the ablation of concrete. (units = W)

CAV-QSURF.n	/cp/	Heat loss from the surface of debris in cavity n. It may go to either a pool or the atmosphere in the bounding control volume. (units = W)
CAV-TGASMOL.n	/c/	Total moles of gas released from cavity n. (units = mol)
CAV-R.n.i	/cp/	Radial coordinate of i-th body point in cavity n. (units = m) Available as a plot variable if and only if the SHAPEPLOT flag has been set on a CAVnnak record (see the description of this flag in Section 2.1). Note the order of the indices.
CAV-Z.n.i	/cp/	Axial coordinate of I-th body point in cavity n. (units = m) Available as a plot variable if and only if the SHAPEPLOT flag has been set on a CAVnnak record (see the description of this flag in Section 2.1). Note the order of the indices.
CAV-CPUT	/p/	Total CPU time used in Cavity package, including computation and I/O. (units = s)
CAV-CPUC	/p/	CPU time used for computation in Cavity package. (units = s)

Partial coding has been included for several other plot variables. The names CAV-DHTOT.n, CAV-HEX.n, CAV-MABLA.n, CAV-MSRC.n, and CAV-RUPALT.n will be recognized by the plot program, but the values plotted will be identically zero.

5. Example Input

Two examples are included in this section. The first example shows typical input for a calculation that begins with an empty cavity and then receives mass from the core package during the calculation, while the second example shows typical input for a calculation that is initiated with mass in the cavity.

5.1 Example for Normal Cavity Input

In this example, cavity 1 is associated with control volume number 201 and is named Cavity 1. It is empty at the start of the calculation but receives mass after the core melts through the vessel lower head. The molten core is transferred from the core package to the Cavity package using the Transfer Process package; CAV receives the debris through “out” transfer process number 102. CORCON type 2 concrete (limestone/common sand) is specified in this example and 13.5% reinforcing steel is included. The initial cavity is a flat-bottomed cylinder with a radius of 3.0 m and a depth of 5.0 m. The cavity is defined with 95 points, of which 10 are initially on the bottom and 10 on the 0.1 m radius transition between bottom and side. The emissivity of the metal layer is changed from the default value to 0.7.

```
*****    CAVITY INPUT    *****
CAV0100   201   'CAVITY 1'
**  Concrete type  **
CAV01C0   CORCON  2             * Concrete type
CAV01C2   FE  0.135             * Include rebar
**  Cavity geometry  **
CAV01G0   CORCON  2             * Geometry type
*         NRAYS   RO     ZO
CAV01G1   95      0.0    0.5
*         ZT   RAD  HIT  RADC  RW   HBB   NBOT NCORN
CAV01G2   0.0  3.0  5.0  0.1   4.0  2.0   10   10
**  Transfer process to introduce debris **
CAV01TP   102                   * RN will use TP 602
**  Miscellaneous parameters  **
CAV01Y1   EMISS.MET  0.7
*****    END OF CAVITY INPUT    *****
```

Input to the Transfer Process package will be required in the form

```
TPOT10200    5    101  UIN.103   * Transfer process for debris
TPM1030000   5    6              * Translation matrix
TPM1030001   1/1  1.0   2/2  1.0   3/3  1.0   4/4  1.0   5/5  1.0
TPOT60200    15   601  DEF.1     * Transfer process for RN
```

where it is assumed that the Core package uses "in" Transfer process 101 and that RN is active with the default 15 classes. For further discussion, see the TP, RN, and COR Users' Guides.

By default, the debris will form a single mixed layer. Complete stratification (the CORCON-Mod2 model) may be enforced by including the record

```
CAV01XA 0.0   * suppress mixing of phases
```

Alternatively, a mechanistic calculation of mixing and reseparation may be specified by including the record

```
CAV01XA 1.0   * perform mechanistic mixing calculation
```

When and if the debris has eroded through the two meters of concrete below cavity 1, the MELCOR calculation will be terminated. It may be restarted by including the record

```
CAV01RA -2     * ignore axial rupture
```

and will then continue as if there were infinite concrete available. If the user desires that the debris fall into a second cavity and the calculation continue, the record

```
CAV01RA 7      * axial rupture with overflow to cavity 7
```

should be included in MELGEN input, along with complete input for cavity 7. (MELGEN must run because a cavity cannot be added on restart.)

5.2 Stand-Alone Cavity Example

This example shows typical input for a “stand-alone” cavity calculation. As in the previous example, cavity 1 is associated with control volume 201, but in this example, the calculation begins with mass present in the cavity. Two layers are initially present: an oxide layer and a metal layer. Both layers are initially at 2500°K. Basalt concrete is specified, but the composition is modified slightly from the default composition, the initial temperature is raised to 350°K, and the ablation temperature is changed to 1773°K (1500°C). The initial cavity geometry is as in the preceding case.

```
*****    CAVITY INPUT    *****
CAV0100   201    'CAVITY 1'
**  Initial layer contents  **
CAV0110   TEMP   2500.
CAV0111   UO2    100000.   ZRO2 14000.
CAV0112   FEO    6000.
CAV0120   TEMP   2500.
CAV0121   ZR 10000.    FE   70000.
CAV0122   CR 10000.    NI   6000.
**  Concrete input  **
CAV01C0   BASALT             * Concrete type
CAV01C1   H2OEVAP 0.060      * Water content
CAV01C2   SIO2   0.700       * SiO2 content
CAV01CA   TINCT  350.0       * Initial concrete temperature
CAV01CB   TABLCT 1773.0      * Ablation temperature
**  Cavity geometry  **
CAV01G0 CORCON    2          * Geometry type
*        NRAYS  RO    ZO
CAV01G1  95     0.0   0.5
*        ZT    RAD   HIT   RADC  RW    HBB   NBOT  NCORN
CAV01G2  0.0   3.0   5.0   0.1   4.0   2.0   10    10
*****    END OF CAVITY INPUT    *****
```

Input must be provided for control volume 201, from which temperature and pressure boundary conditions for the cavity will be obtained. These properties may be directly specified as tabular functions of time by treating this volume as a “time-specified volume.” See the Control Volume Hydrodynamics Users’ Guide for details.

By default, the initial debris will be placed in a single, mixed-phase layer, *despite the definition of separate metallic and oxidic layers*. The treatment of mixing may be modified by input for the MIXING keyword on a CAV01ak record, as described in the previous example.

6. Discussion of Output

The Cavity package output should be self-explanatory. Basically, each edit identifies the cavity, its associated control volume, and the status of the cavity (“sleeping” if there is no material presently in cavity, “active” if material is currently present). This is followed by a summary of the major CORCON options in effect and, if the cavity is active, by detailed output (in CORCON format) in several sections as described in the CORCON Reference Manual. This output includes:

(1) A general summary giving the pool configuration, maximum depth and radius, an approximate energy budget, and checks on conservation of mass and energy. As noted in CORCON documentation, the energy budget is approximate, and should not be expected to balance exactly. The entry for “changes in pool enthalpy” contains latent heats, and may be significant at times when the pool temperature is nearly constant, but the freezing point of a layer is changing as a result of changing composition. MELCOR calculations frequently require a far larger number of timesteps than do calculations with stand-alone CORCON. Therefore, the errors in mass and energy conservation may become larger than a user is accustomed to seeing. Simple accumulation of roundoff would lead to relative errors of approximately SQRT(n) times unit roundoff after n timesteps. This would be roughly 10^{-11} on a typical 64-bit machine or 10^{-4} on a typical 32-bit machine after 10^4 steps.

(2) Gas generation results, giving generation rates and cumulative releases, both as masses and in moles. Because generation of trace gases has been suppressed, only the major species H_2O, H_2, CO_2, and CO are included.

(3) Geometry of the cavity. Information includes the locations of body points defining the cavity, inclinations of the walls, locations of layer interfaces, and local void fractions.

(4) Details of heat transfer at the interface between the debris pool and the concrete. This includes ablation rates, thickness of the gas film, and temperature of the pool/film interface.

(5) Results of chemical reactions during the timestep.

(6) Pool composition.

(7) Layer properties, including thermochemical and transport properties of each (occupied) layer. Gas-bubble and layer-oriented heat transfer results including crust-model quantities are also given, as are important terms in the energy equation for each layer.

(8) Properties of the individual phases in mixed-phase (HMX or LMX) layers, if present, including mass, density, and melting range.

If the cavity is inactive, the first edit for each calculation will still include geometric and other relevant data. In any case, it will be followed by a summary of concrete properties, including the composition, the composition of reinforcing bar (if present), the melt range, the ablation temperature, and the heat of ablation.

7. Diagnostic and Error Messages

Diagnostic and error messages may be printed either in MELGEN or in MELCOR. Messages resulting from errors or unrecognized records in user input to MELGEN include the record identifier and sufficient information to allow the user to identify the error. Error messages may be printed during the subsequent calculation of rates in MELGEN or during execution of MELCOR to warn of possibly inaccurate results or indicate the cause of problem termination.

The CORCON manual lists a number of nonfatal errors involving such things as failure of the crust model to converge within the requested tolerance. Because an alternate treatment is provided, and conservation laws are *not* violated, the default treatment in MELCOR is not to print these messages except to the extended diagnostic file, which is primarily of interest to code developers. In any case, there is little or nothing that a code user can (or should) do about them. See the WARNINGLEVEL input record in the Executive (EXEC) Package Users' Guide; the messages referred to above have been given a severity level of 3.

There are also several errors beyond which the code cannot continue, and the calculation will be stopped after a restart dump is written. These errors include the appearance of a singular matrix in the chemical equilibrium routine CCMLTR or in the heat transfer/energy conservation routines CCENR1, CCENR2, CCHLAY, or CCINTP. The first of these has been reported, the others have not. The user's only option is to restart the calculation with some modification to input—a change in timestep is frequently sufficient—to try to avoid the error. It may be necessary to pick the calculation up from an earlier restart rather than the final one.

Another set of fatal errors includes failure in the iterative determination of layer temperatures in subroutine CCTMPF, which is called from subroutines CCENR1 and

CCPLAY, or of boundary layer heat transfer in subroutine CCFILM. Here, also, the user's only option is usually to restart the calculation with some input modification. In the former case (involving subroutine CCTMPF), the printed output should first be checked to assure that the debris temperatures are reasonable. If they are not, the problem may have been caused by an error in definition of the heat source in CAV, and the associated input and output should be checked carefully.

In the interest of completeness, we note that there are a number of additional points in the Cavity package coding where execution will be terminated if an apparent corruption of the database is detected. Examples include, but are not limited to, the overwriting of table bounds in expansion of specific heat tables in subroutine CCCFND (because the array dimensions are adequate), or the appearance of mass in a mixed-phase layer (because there is no provision for creating such a layer in CAV). Several nonfatal messages not mentioned in this section, such as a warning that the emissivity tables in subroutine CCEMIS are being extrapolated (because the CAV package does not allow the table option in CORCON) can only result from corruption of the database. Unfortunately, it was determined that these terminations would not be executed or the warnings issued (short of a machine error) in distributed versions of MELCOR. Therefore, if one should be encountered (and is reproducible), *the user must first eliminate the possibility that it resulted from an error in a local modification to the code*. If it can be demonstrated that this is *not* the case, the only recourse is to contact the code development team.